

# SELF-CONSISTENT SEPARABLE RPA FOR DENSITY- AND CURRENT-DEPENDENT FORCES

J. Kvasil<sup>1</sup>, V.O. Nesterenko<sup>2</sup>, and P.-G. Reinhard<sup>3</sup>

<sup>1</sup> Institute of Particle and Nuclear Physics, Charles University,  
V.Holešovičkách 2, CZ-18000 Praha 8, Czech Republic  
E-mail: kvasil@ipnp.troja.mff.cuni.cz

<sup>2</sup> BLTP, Joint Institute for Nuclear Research 141980, Dubna, Moscow  
Region, Russia  
E-mail: nester@thsun1.jinr.ru

<sup>3</sup> Institut für Theoretische Physik, Universität Erlangen, W-8520 Erlangen,  
Germany  
E-mail: mpt218@theorie2.physik.uni-erlangen.de

## ABSTRACT

Self-consistent factorization of two-body residual interaction is proposed for arbitrary density- and current-dependent energy functionals. Following this procedure, a separable RPA (SRPA) method is constructed. SRPA dramatically simplifies the calculations and demonstrates quick convergence to exact results. The method is tested for SkM\* forces.

# 1 Introduction

Effective nucleon-nucleon interactions (Skyrme, Gogny, ...) are widely used for description of nuclear properties (see, for example, Ref.[1]). However, their application to nuclear dynamics is rather limited even in the linear regime. The latter is usually treated within random-phase-approximation (RPA) and assumes diagonalization of matrices with the rank determined by the size of the particle-hole ( $ph$ ) configuration space. In deformed and heavy spherical nuclei this space is impressive and condemns to a huge computational effort. As a result, the effective forces are mainly applied to study ground state properties while RPA calculations are very limited.

RPA problem becomes much simpler if the residual two-body interaction is factorized (reduced to a separable form):

$$\sum_{mnij} \langle mn|V_{res}|ij \rangle a_m^+ a_n^+ a_j a_i \rightarrow \sum_{k,k'=1}^K \kappa_{k,k'} \hat{X}_k \hat{X}_{k'},$$

$$\hat{X}_k = \sum_{ph} \langle p|\hat{X}_k|h \rangle a_p^+ a_h. \quad (1)$$

This allows to avoid dealing with high-rank matrices. The main trouble is to accomplish the factorization self-consistently, with minimal number of separable terms and high accuracy.

Factorization of the residual interaction is widely used in nuclear theory but mainly within trivial schemes exploiting one separable term with an intuitive guess for the separable one-body operator  $\hat{X}$ . The strength constant  $\kappa$  is usually fitted so as to reproduce available experimental data (see e.g. [2]). The separable interaction thus obtained does not depend on nuclear density and is not consistent with the mean field. Obviously, accuracy and predictability of such schemes are rather low. Several self-consistent schemes<sup>3-8</sup> proposed during last decades signified a certain progress in this problem. However, these schemes were not sufficiently general. Some of them were limited to analytic or simple numerical estimates<sup>3-6</sup> the others were not fully self-consistent [7] or covered only particular effective forces [8].

In the present paper we propose a general self-consistent separable RPA (SRPA) approach relevant to arbitrary density- and current-dependent functionals. The self-consistent scheme of Ref.[5] is generalized to the case of several separable operators. The operators have maxima at different slices

of the nucleus, which is crucial for accurate reproduction of  $V_{res}$  and high numerical accuracy. SRPA is tested for the case of SkM\* functional [9].

## 2 General formulation of SRPA

The nucleus is assumed to undergo small-amplitude harmonic vibrations around HF or HFB ground state. The starting point is a general time-dependent energy functional  $E(J_s^\alpha(\vec{r}, t))$  depending on a set of arbitrary neutron and proton densities and currents  $J_s^\alpha(\vec{r}, t)$  ( $s = n, p$ ;  $\alpha$  labels densities and currents)

$$E(J_s^\alpha(\vec{r}, t)) = \langle \Psi(t) | \hat{H} | \Psi(t) \rangle = \int \mathcal{H}(\vec{r}) d\vec{r} \quad (2)$$

where  $|\Psi(t)\rangle$  is the wave function of the vibrating system described as the time-dependent Slater determinant. Time-dependent densities and currents are determined through the corresponding operators as

$$J_s^\alpha(\vec{r}, t) = \langle \Psi(t) | \hat{J}_s^\alpha(\vec{r}) | \Psi(t) \rangle. \quad (3)$$

The wave function  $|\Psi(t)\rangle$  is obtained from the static HF Slater determinant  $|\Psi_0\rangle$  by the scaling transformation [5]

$$|\Psi(t)\rangle = \prod_{k=1}^K \exp[-i(q_{sk}(t) - \langle q_{sk} \rangle) \hat{P}_{sk}] \exp[-ip_{sk}(t) \hat{Q}_{sk}] |\Psi_0\rangle \quad (4)$$

where  $\hat{Q}_{sk}$  and  $\hat{P}_{sk}$  are, respectively, T-even and T-odd generators fulfilling the equations

$$\begin{aligned} \hat{Q}_{sk}^+ &= \hat{Q}_{sk}, & T \hat{Q}_{sk} T^{-1} &= \hat{Q}_{sk}, & [\hat{H}, \hat{Q}_{sk}] &\equiv -i \hat{P}_{sk}, \\ \hat{P}_{sk}^+ &= \hat{P}_{sk}, & T \hat{P}_{sk} T^{-1} &= -\hat{P}_{sk}, & [\hat{H}, \hat{P}_{sk}] &\equiv -i \hat{Q}_{sk} \end{aligned} \quad (5)$$

and  $q_{sk}(t)$  and  $p_{sk}(t)$  are the corresponding T-even and T-odd harmonic deformations given by

$$\begin{aligned} q_{sk}(t) &\equiv \langle \Psi(t) | \hat{Q}_{sk} | \Psi(t) \rangle, & p_{sk}(t) &\equiv \langle \Psi(t) | \hat{P}_{sk} | \Psi(t) \rangle, \\ & & \langle q_{sk} \rangle &\equiv \langle \Psi_0 | \hat{Q}_{sk} | \Psi_0 \rangle. \end{aligned} \quad (6)$$

The HF single-particle Hamiltonian is

$$\hat{h}_0(\vec{r}) = \sum_{\alpha,s} \frac{\partial \mathcal{H}(J_n^\alpha, J_p^\alpha)}{\partial J_s^\alpha} \hat{J}_s^\alpha(\vec{r}). \quad (7)$$

Using the scaling (4), it is straightforward to find time-dependent density and current variations

$$\begin{aligned} J_s^\alpha(\vec{r}, t) &\simeq J_s^\alpha(\vec{r}) + \delta J_s^\alpha(\vec{r}, t), \\ \delta J_s^\alpha(\vec{r}, t) &= \langle \Psi(t) | \hat{J}_s^\alpha | \Psi(t) \rangle - \langle \Psi_0 | \hat{J}_s^\alpha | \Psi_0 \rangle = \\ &= -i \sum_k \sum_{s=n,p} \{ (q_{sk}(t) - \langle q_{sk} \rangle) < | [\hat{P}_{sk}, \hat{J}_s^\alpha(\vec{r})] | > \\ &\quad + p_{sk}(t) < | [\hat{Q}_{sk}, \hat{J}_s^\alpha(\vec{r})] | > \} \end{aligned} \quad (8)$$

and the response Hamiltonian (vibrating single-particle potential)

$$\begin{aligned} \hat{h}(\vec{r}, t) &\simeq \hat{h}_0(\vec{r}) + \hat{h}_{res}(\vec{r}, t), \\ \hat{h}_{res}(\vec{r}, t) &= \sum_{\alpha's'} [\frac{\partial \hat{h}_0(\vec{r})}{\partial J_{s'}^\alpha}] \delta J_{s'}^{\alpha'}(\vec{r}, t) = \sum_{\alpha s} \sum_{\alpha's'} [\frac{\partial^2 \mathcal{H}(\vec{r})}{\partial J_s^\alpha \partial J_{s'}^{\alpha'}}] \delta J_{s'}^{\alpha'}(\vec{r}, t) \hat{J}_s^\alpha(\vec{r}) \\ &= \sum_{sk} \{ (q_{sk}(t) - \langle q_{sk} \rangle) \hat{X}_{sk}(\vec{r}) + p_{sk}(t) \hat{Y}_{sk}(\vec{r}) \}. \end{aligned} \quad (9)$$

In the above equations we introduced one-body operators

$$\begin{aligned} \hat{X}_{sk}(\vec{r}) &= i \sum_{s'\alpha'\alpha} [\frac{\partial^2 \mathcal{H}}{\partial J_{s'}^{\alpha'} \partial J_s^\alpha}] < | [\hat{P}_{sk}, \hat{J}_s^\alpha] | > \hat{J}_{s'}^{\alpha'}(\vec{r}), \\ \hat{Y}_{sk}(\vec{r}) &= i \sum_{s'\alpha'\alpha} [\frac{\partial^2 \mathcal{H}}{\partial J_{s'}^{\alpha'} \partial J_s^\alpha}] < | [\hat{Q}_{sk}, \hat{J}_s^\alpha] | > \hat{J}_{s'}^{\alpha'}(\vec{r}) \end{aligned} \quad (10)$$

where  $\hat{X} = \hat{X}^+$  is T-even,  $\hat{Y} = \hat{Y}^+$  is T-odd, and the notation

$$< [\hat{A}, \hat{B}] > = \langle \Psi_0 | [\hat{A}, \hat{B}] | \Psi_0 \rangle \quad (11)$$

is used. The moments of the operators are

$$\begin{aligned} \langle \delta \hat{X}_{sk}(t) \rangle &\equiv \langle \Psi(t) | \hat{X}_{sk} | \Psi(t) \rangle - \langle \Psi_0 | \hat{X}_{sk} | \Psi_0 \rangle = \\ &= i \sum_{s'k'} (q_{s'k'}(t) - \langle q_{s'k'} \rangle) < | [\hat{P}_{s'k'}, \hat{X}_{sk}] | > = \\ &\equiv \sum_{s'k'} (q_{s'k'}(t) - \langle q_{s'k'} \rangle) \kappa_{sk, s'k'}^{-1} \end{aligned} \quad (12)$$

$$\begin{aligned}
\langle \delta \hat{Y}_{sk}(t) \rangle &\equiv \langle \Psi(t) | \hat{Y}_{sk} | \Psi(t) \rangle - \langle \Psi_0 | \hat{Y}_{sk} | \Psi_0 \rangle = \\
&= i \sum_{s'k'} p_{s'k'}(t) \langle [ \hat{P}_{s'k'}, \hat{Y}_{sk} ] \rangle = \\
&\equiv \sum_{s'k'} p_{s'k'}(t) \eta_{sk,s'k'}^{-1}
\end{aligned} \tag{13}$$

where we introduced the inverse strength matrices

$$\begin{aligned}
\kappa_{sk,s'k'}^{-1} &= \kappa_{s'k',sk}^{-1} = -i \langle [ \hat{X}_{sk}, \hat{P}_{s'k'} ] \rangle = \\
&= \int d\vec{r} \sum_{\alpha\alpha'} \left[ \frac{\delta^2 \mathcal{H}}{\delta J_{s'}^{\alpha'} \delta J_s^{\alpha}} \right] \langle [ \hat{J}_s^{\alpha}, \hat{P}_{sk} ] \rangle < [ \hat{J}_{s'}^{\alpha'}, \hat{P}_{s'k'} ] \rangle,
\end{aligned} \tag{14}$$

$$\begin{aligned}
\eta_{sk,s'k'}^{-1} &= \eta_{s'k',sk}^{-1} = -i \langle [ \hat{Y}_{sk}, \hat{Q}_{s'k'} ] \rangle = \\
&= \int d\vec{r} \sum_{\alpha\alpha'} \left[ \frac{\delta^2 \mathcal{H}}{\delta J_{s'}^{\alpha'} \delta J_s^{\alpha}} \right] \langle [ \hat{J}_s^{\alpha}, \hat{Q}_{sk} ] \rangle < [ \hat{J}_{s'}^{\alpha'}, \hat{Q}_{s'k'} ] \rangle.
\end{aligned} \tag{15}$$

Harmonic collective shifts  $q_{sk}(t) - \langle q_{sk} \rangle$  and velocities  $p_{sk}(t)$  read as

$$\begin{aligned}
q_{sk}(t) - \langle q_{sk} \rangle &= \bar{q}_{sk} \cos(\omega t) = \frac{1}{2} \bar{q}_{sk} (e^{i\omega t} + e^{-i\omega t}), \\
p_{sk}(t) &= \bar{p}_{sk} \sin(\omega t) = \frac{1}{2i} \bar{p}_{sk} (e^{i\omega t} - e^{-i\omega t}).
\end{aligned} \tag{16}$$

Following the Thouless theorem, the perturbed wave function (7) can be also written as

$$| \Psi(t) \rangle \sim (1 + \sum_{ph} c_{ph}(t) a_p^\dagger a_h) | \Psi_0 \rangle \tag{17}$$

where  $c_{ph}(t)$  are the time-dependent particle-hole contributions to the given excited state. Substituting (17) into the time-dependent HF equation

$$i \frac{d}{dt} | \Psi(t) \rangle = (\hat{h}_0 + \hat{h}_{res}(t)) | \Psi(t) \rangle \tag{18}$$

and using

$$c_{ph}(t) = c_{ph}^+ e^{i\omega t} + c_{ph}^- e^{-i\omega t}, \tag{19}$$

one gets the relation between  $c_{ph}^\pm$  and collective deformations  $\bar{q}_{sk}$  and  $\bar{p}_{sk}$

$$c_{ph\epsilon s}^\pm = -\frac{1}{2} \frac{\sum_k [\bar{q}_{sk} \langle p | \hat{X}_{sk} | h \rangle \mp i \bar{p}_{sk} \langle p | \hat{Y}_{sk} | h \rangle]}{\varepsilon_{ph} \pm \omega}, \tag{20}$$

where  $\varepsilon_{ph} = \varepsilon_p - \varepsilon_h$ ,  $\varepsilon_p$  and  $\varepsilon_h$  are the particle and hole energies, respectively.

In addition to Eqs. (12)-(13), the moments  $\langle \delta \hat{X}_{sk}(t) \rangle$  and  $\langle \delta \hat{Y}_{sk}(t) \rangle$  can be also expressed in terms of the Thouless wave function (16):

$$\begin{aligned} \langle \delta \hat{X}_{sk}(t) \rangle &= \sum_{ph} (c_{ph}(t))^* \langle p | \hat{X}_{sk} | h \rangle + c_{ph}(t) \langle h | \hat{X}_{sk} | p \rangle, \\ \langle \delta \hat{Y}_{sk}(t) \rangle &= \sum_{ph} (c_{ph}(t))^* \langle p | \hat{Y}_{sk} | h \rangle + c_{ph}(t) \langle h | \hat{Y}_{sk} | p \rangle. \end{aligned} \quad (21)$$

Then, using Eq. (20) an equating the moments (12)-(13) and (21), we obtain the system of equations for unknowns  $\bar{q}_{sk}$  and  $\bar{p}_{sk}$ :

$$\begin{aligned} \sum_{s'k'} \bar{q}_{s'k'} [S_{s'k',sk}(XX) - \kappa_{s'k',sk}^{-1}] + \sum_{s'k'} \bar{p}_{s'k'} S_{s'k',sk}(XY) &= 0, \\ \sum_{s'k'} \bar{q}_{s'k'} S_{s'k',sk}(XY) + \sum_{s'k'} \bar{p}_{s'k'} [S_{s'k',sk}(YY) - \eta_{s'k',sk}^{-1}] &= 0 \end{aligned} \quad (22)$$

with

$$\begin{aligned} S_{s'k',sk}(XX) &= \sum_{ph} \frac{1}{\varepsilon_{ph}^2 - \omega^2} \{ \langle p | \hat{X}_{s'k'} | h \rangle^* \langle p | \hat{X}_{sk} | h \rangle (\varepsilon_{ph} - \omega) \\ &\quad + \langle p | \hat{X}_{s'k'} | h \rangle \langle p | \hat{X}_{sk} | h \rangle^* (\varepsilon_{ph} + \omega) \}, \\ S_{s'k',sk}(YY) &= \sum_{ph} \frac{1}{\varepsilon_{ph}^2 - \omega^2} \{ \langle p | \hat{Y}_{s'k'} | h \rangle^* \langle p | \hat{Y}_{sk} | h \rangle (\varepsilon_{ph} - \omega) \\ &\quad + \langle p | \hat{Y}_{s'k'} | h \rangle \langle p | \hat{Y}_{sk} | h \rangle^* (\varepsilon_{ph} + \omega) \}, \\ S_{s'k',sk}(XY) &= -i \sum_{ph} \frac{1}{\varepsilon_{ph}^2 - \omega^2} \{ \langle p | \hat{X}_{s'k'} | h \rangle^* \langle p | \hat{Y}_{sk} | h \rangle (\varepsilon_{ph} - \omega) \\ &\quad + \langle p | \hat{X}_{s'k'} | h \rangle \langle p | \hat{Y}_{sk} | h \rangle^* (\varepsilon_{ph} + \omega) \}. \end{aligned} \quad (23)$$

The matrix of the system (22) is symmetric and real. By equating the determinant of the system to zero,  $\det D = 0$ , we get the dispersion equation for eigenvalues  $\omega_\nu$ .

It can be shown that the same equations can be obtained through the standard RPA equations with the Hamiltonian

$$\hat{H}_{RPA} = \hat{h}_0 + \hat{V}_{res}, \quad (24)$$

where

$$\hat{V}_{res} = -\frac{1}{2} \sum_{sk} \sum_{s'k'} [\tilde{\kappa}_{sk,s'k'} \hat{X}_{sk} \hat{X}_{s'k'} + \tilde{\eta}_{sk,s'k'} \hat{Y}_{sk} \hat{Y}_{s'k'}]. \quad (25)$$

The strength constants  $\tilde{\kappa}$  and  $\tilde{\eta}$  are obtained by inversion of the matrices (14) and (15).

Eqs. (10), (14), (15), (20), (22), (23) constitute the set of SRPA equations.

The rank of SRPA matrix (22) is  $4K$  with  $K = 3 - 6$  (see next section). So, high-rank matrix of exact RPA shrinks to low-rank SRPA matrix. This minimizes the computational effort. At the same time, as is demonstrated below, SRPA provides high accuracy of the calculations.

The approach is fully self-consistent and does not need any adjusting parameters in addition to the starting functional. Unlike the trivial separable schemes, SRPA gives analytical expressions for both separable operators and strength constants. Relative contributions of different separable operators are self-consistently regulated for every RPA state.

### 3 SRPA test with Skyrme functional

SRPA was tested for the particular case of SkM\* functional [9]. Isoscalar and isovector densities (nucleon, kinetic, spin and spin-orbital) and currents have been involved. The strength function

$$b_L(X\lambda, gr \rightarrow \omega) = \sum_{\nu} \omega_{\nu}^L < \nu | \hat{\mathcal{M}}(X\lambda) | 0 >^2 \rho(\omega - \omega_{\nu}) \quad (26)$$

with Lorentz weight  $\rho(x - y) = \frac{1}{2\pi} \frac{\Delta}{(x-y)^2 + (\Delta/2)^2}$  ( $\Delta = 1$  MeV is the averaging parameter) has been calculated for isoscalar E2 and isovector E1 transitions in  $^{40}\text{Ca}$  and  $^{208}\text{Pb}$  and compared with the results of exact RPA. In (26),  $\hat{\mathcal{M}}(X\lambda)$  is operator of  $X\lambda$ -transition.

The set of  $K = 2$  generators

$$\hat{Q}_k(\vec{r}) = R_k(r)(Y_{\lambda\mu} + h.c.), \quad \hat{P}_k = i[\hat{H}, \hat{Q}_k] \quad (27)$$

has been used with  $R_1(r) = r^{\lambda}$ ,  $R_2(r) = r^{\lambda+2}$ . The first  $Q_k$ -generator coincides with the corresponding  $E\lambda$ -transition operator in the long-wave approximation, and the other creates operators  $\hat{X}_{sk}$  and  $\hat{Y}_{sk}$  with maxima in the interior.

The comparison between SRPA and exact RPA results is exhibited in Fig. 1. Already first operator gives excellent description of E2 giant resonance. However, it is not enough to reproduce E1 data. The second operator considerably improves the agreement and provides a satisfactory description.

## 4 Conclusions

A general procedure for self-consistent factorization of the residual interaction is proposed for arbitrary density- and current-dependent functionals. The separable RPA (SRPA) constructed in the framework of this approach dramatically simplifies the calculations while keeping high accuracy of numerical results. The latter was demonstrated for the case of SkM\* functional.

SRPA can be used for description of  $E\lambda$  and  $M\lambda$  response in both spherical and deformed nuclei. In the case of deformed nuclei it allows to take into account the coupling between electric and magnetic modes. The approach can serve as a good basis for anharmonic corrections, description of vibrational states in odd and odd-odd nuclei. SRPA can be especially useful for investigation of dynamics of deformed nuclei where applications of effective forces (Skyrme, Gogny, ...) are very scarce. One of the most promising lines of future studies is dynamics of exotic nuclei obtained in radioactive beams.

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FIGURE CAPTIONS:

**Figure 1.** Isoscalar  $E2$  and isovector  $E1$  strength functions in  $^{40}\text{Ca}$  and  $^{208}\text{Pb}$ . The lines represent exact RPA results (full) and SRPA ones with one (dotted) and two (dashed) operators.